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RESEARCH REPORT No. CX-43

Upper Bounds on Scattering Lengths for Static Potentials

LARRY SPRUCH and LEONARD ROSENBERG

Contract No. AF 19(604)4555
OCTOBER, 1959

CX-43
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The research reported in this paper has been sponsored by the Geophysics Research Directorate of the Air Force Cambridge Research Center, Air Research and Development Command, under Contract No. AF 19(604)4555.

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Abstract

It is shown that in the zero energy scattering of a particle by a center of force, where no bound state exists, the Kohn variational principle provides an upper bound on the scattering length. A bound may also be obtained from Hulthén's method, although with the same form of trial function the Kohn result will be lower (and therefore better) than the one obtained from the Hulthén principle. The Rubinow formulation need not provide a bound; for those calculations which have been performed in this form, the results may be converted without any further calculations so that they correspond to the Kohn form, and therefore, under the circumstances considered, do give a bound. Analagous results hold for states of non-zero orbital angular momentum.

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I. INTRODUCTION

Variational methods have proved to be of great value in the theoretical analysis of the problem of the scattering of a particle by a center of force. However, the utility of variational techniques in the more complicated problem of scattering by a compound system is considerably impaired by the fact that it is more difficult, in the many body problem, to construct accurate trial functions, and a variational calculation, using a poor trial function, will generally lead to poor results. In fact, these calculations will only be meaningful when accompanied by an affirmation of validity, using some reliable criterion. It is our purpose to present one such rigorous validity criterion for the case of zero energy scattering. The present discussion will, for the sake of clarity of presentation, be confined to the problem of scattering by a static potential; the generalization to the more interesting problem in which the scatterer is a compound system is given in a paper[1] which will be referred to in the following as II.

The problem of obtaining rigorous bounds on the error made in a variational calculation for the scattering by a center of force has been considered previously by a number of authors[2,3]; perhaps the most satisfying solution is that due to Kato[3]. As a special case of the Kato method, it has been shown[4] that if no bound state exists for the potential considered, then the Kohn variational principle[5] provides an upper bound on the scattering length. Since the scattering length is one of the two parameters which completely characterize the low energy scattering in the shape independent approximation, its

determination is of great importance. The proof involves an application of a theorem proved by Levinson[6]. In Section II, an alternate proof, entirely independent of the Kato method, will be presented. The advantage of this alternate proof, in addition to its directness and simplicity, lies in the fact that its generalization to the case of scattering by a compound system is straightforward. On the other hand, using the Kato approach, one encounters the difficulty that a rigorous proof of the generalization of Levinson's theorem to the many body problem has not been given. Indeed, in the case where there are identical particles in the system, the statement of the theorem cannot be taken as a direct extension of the one given by Levinson, but rather requires some modification. (This problem has been considered by Swan[7] who presents a proof of a theorem which takes into account the modification required by the Pauli principle. However, the basic equation studied by Swan is the one appropriate to the static approximation and the general proof has not been given.) Further, the generalization of the Kato formalism itself to include the effects of the Pauli principle has not been made; there are certain difficulties here which do not arise in the case of scattering by a compound system with no identical particles (though it appears that there exist some cases, at least, where these difficulties could be circumvented).

Under the circumstances considered, namely zero energy scattering with no bound states, it is found that the Hulthén variational principle[8], as well as the Kohn principle, gives an upper bound on

the scattering length. The Born approximation also provides an upper bound, since it may be derived from the Kohn principle. While the Rubinow formulation[9] need not give a bound, for those calculations that have been performed in the Rubinow form, it is a trivial matter to convert the results to the Kohn form, thereby obtaining a bound. A numerical example, using a square well potential with a repulsive core, is presented in Section III to illustrate some of these points. The extension to the case of higher angular momenta is presented in Section IV.

II. THE STATIC PROBLEM

The zero energy scattering of a particle of mass m in a static central potential, $V(r)$, is described by a function, $u_i(r)$, the true partial wave of zero orbital angular momentum, which satisfies the differential equation

$$\mathcal{L} u_i(r) \equiv \left[\frac{d^2}{dr^2} + W(r) \right] u_i(r) = 0 \quad ,$$

$$W(r) \equiv -(2m/\hbar^2)\, V(r).$$

The subscript i will be used to distinguish between the two standard types of assumed boundary conditions:

$$u_i(0) = 0 \quad , \qquad i = 1,2 \quad ,$$

$$u_1(r) \to A - r \quad , \qquad \text{for } r \to \infty \quad ,$$

$$u_2(r) \to 1 - r/A \quad , \qquad \text{for } r \to \infty \quad .$$

Here A is the scattering length, which is related to the zero energy

cross section, $\sigma(k = 0)$, by

$$\sigma(k = 0) = 4\pi A^2 \quad .$$

The connection between the scattering length and the zero angular momentum phase shift, η, at zero energy is

$$-A^{-1} = (k \cot \eta)_{k=0} \quad .$$

We now introduce two trial functions, u_{it}, $(i = 1,2)$, satisfying the boundary conditions

$$u_{it}(0) = 0 \quad , \qquad i = 1,2 \quad ,$$

$$u_{1t}(r) \to A_t - r \quad , \qquad \text{for } r \to \infty \quad ,$$

$$u_{2t}(r) \to 1 - r/A_t \quad , \qquad \text{for } r \to \infty \quad ,$$

where A_t, the trial scattering length, is an arbitrary constant which may in fact be chosen differently in u_{1t} and u_{2t}. It will always be assumed that $u_{it}(r)$ is continuous and has a continuous first derivative. With $w_i(r)$ defined by

$$w_i(r) = u_{it}(r) - u_i(r) \quad , \qquad i = 1,2 \quad ,$$

the Kato identity for zero energy scattering, taking the alternate forms

$$A = A_t - \int u_{1t} \mathcal{L} u_{1t} \, dr + \int w_1 \mathcal{L} w_1 \, dr \quad , \qquad (2.1)$$

and

$$-A^{-1} = -A_t^{-1} - \int u_{2t} \mathcal{L} u_{2t} \, dr + \int w_2 \mathcal{L} w_2 \, dr \quad , \qquad (2.2)$$

may be shown to hold. (All integrals will be understood to have the

limits zero and infinity).

The above results will be rederived in Section IV in a form valid for partial waves of arbitrary angular momentum. If, in Eqs. (2.1) and (2.2), the second order term, $\int w_i \mathcal{L} w_i \, dr$, is dropped, two different forms of the variational principle for the scattering length are obtained. Kato goes further; his method, which is applicable to non-zero energies as well, is concerned with obtaining bounds on the second order term, thereby providing bounds on A (or $k \cot \eta$ for $k \neq 0$). While we will use the Kato identity in its zero energy form, Eqs. (2.1) and (2.2), it is noted that the Kato method for obtaining bounds on $\int w_i \mathcal{L} w_i \, dr$ will not be used at all in the present paper.

Rather, as will now be shown, in the particular case where the potential cannot support a bound state, we have the simple result that

$$\int w_1 \mathcal{L} w_1 \, dr = -(2m/\hbar^2) \int w_1 H w_1 \, dr \leq 0 \quad , \qquad (2.3)$$

where H is the reduced Hamiltonian of the system. (The case i = 2 will be considered later).

Before proceeding to the proof we wish to distinguish between the two separate reasons for which the present method is restricted to the case where no bound states exist. Firstly, if a bound state is possible the competing process of capture with the emission of a gamma ray is possible and the effect of the center of force on the incident beam of zero energy cannot be completely characterized by a single real scattering length. This is not the essential point, however, since the approximation of ignoring the radiative capture process is often an

extremely good one, and we have been able to develop methods which, to the extent that this approximation is in fact valid, do provide rigorous upper bounds on the scattering length. (A report of this work has been submitted for publication.) However, Eq. (2.3) will not be generally valid in these cases simply because w_1 might contain a sufficient amount of the bound state wave function to make $\int w_1 \mathcal{L} w_1 \, dr$ positive.

To formally prove the inequality, Eq. (2.3), it is first noted that if no bound state exists, $\mathcal{L}$ is a negative definite operator on the space of quadratically integrable functions (i.e., H is positive definite). Now $w_1(r)$ approaches a constant value for large r and is therefore not quadratically integrable. If, however, we define

$$w_1(r,\lambda) \equiv w_1(r)\, e^{-\lambda r} \quad ,$$

we have

$$M_1(\lambda) \equiv \int w_1(r,\lambda)\, \mathcal{L}\, w_1(r,\lambda)\, dr < 0 \ , \quad \lambda > 0.$$

To show that $M_1(0)$ is not positive, it remains to show that $M_1(\lambda)$ is continuous at $\lambda = 0$. This is immediately verified. Thus, we have

$$M_1(\lambda) - M_1(0) = \int w_1(r) \left[e^{-2\lambda r} - 1 \right] \mathcal{L}\, w_1(r)\, dr$$
$$+ \lambda^2 \int w_1^{\,2}(r)\, e^{-2\lambda r}\, dr - 2\lambda \int w_1(r)\, w_1'(r)\, e^{-2\lambda r}\, dr \ .$$

Each of the three terms may be seen to be arbitrarily small, in absolute magnitude, for λ sufficiently small; explicit use is made of

the fact that $|w_1(r)|$ is bounded from above for all $\underline{r}$, and that $w_1'(r) \to 0$ for large $\underline{r}$. The desired inequality has thus been established.

We therefore have the result that if no bound state exists, the scattering length satisfies the relation

$$A \leq A_t - \int u_{1t} \mathcal{L} u_{1t} \, dr \quad , \tag{2.4}$$

with

$$u_{1t}(0) = 0 \quad , \tag{2.5}$$

$$u_{1t}(r) \to A_t - r \quad , \quad \text{for } r \to \infty \quad .$$

The right hand side of Eq. (2.4) corresponds to the Kohn variational approximation to the scattering length and, as we now see, always gives a value which lies above the true scattering length under the specified condition.

While any choice of the parameters in the trial function will lead to a bound on A, we now consider the two particular alternative prescriptions which are widely used in scattering problems for evaluating the variational parameters in a trial function. Assume that the trial function contains N + 1 variational parameters, one of them being the trial scattering length, A_t. If one applies to Eq. (2.4) the method given by Kohn, the N + 1 equations are taken to be

$$\frac{\partial Q}{\partial A_t} = 0 \quad ,$$

$$\frac{\partial Q}{\partial a_n} = 0 \quad , \qquad n = 1, 2, \cdots N \, , \tag{2.6}$$

where

$$Q = A_t - I_1 \quad ,$$

and

$$I_1 = \int u_{1t} \mathcal{L} u_{1t} \, dr \quad .$$

In the method of Hulthén we have

$$I_1 = 0 \, ,$$

$$\frac{\partial I_1}{\partial a_n} = 0 \, , \qquad n = 1, 2, \cdots N \, . \tag{2.7}$$

While in general one cannot know which of these two methods will give better results it is interesting to note that in the type of problem under consideration, namely, zero energy scattering and no bound state, the Kohn method is definitely superior. This follows from the fact that since Q is bounded from below, for a given form of the trial

function the variational parameters evaluated according to Eqs. (2.6) give the <u>smallest</u> value for Q, which therefore provides the closest approximation to the true scattering length. (If the variational parameters do not appear linearly in the trial function, there will in general be more than one solution to Eqs. (2.6). That solution which gives the smallest value for Q should be adopted; it provides the optimum set of values for the parameters.) Further, if a second trial function is used which is more flexible than the first, in such a way that for certain values of the parameters the second form reduces to the first, then an improved result is guaranteed if the Kohn method is used; no such statement can be made in general for the Hulthén method.

We have thus far been considering the results which follow from Eq. (2.1). Turning to Eq. (2.2), we find that an attempt to show, in a similar way, that $\int w_2 \mathcal{L} w_2 \, dr \leq 0$ fails; the proof that

$$\int w_2(r) \, e^{-\lambda r} \mathcal{L} \left[w_2(r) \, e^{-\lambda r} \right] dr$$

is continuous at $\lambda = 0$ does not go through. The reason is that the asymptotic form of $w_2(r)$ is $(A_t^{-1} - A^{-1}) \, r$, which violates one of the conditions under which the continuity was established in the first case. Indeed, the class of functions to which $w_2(r)$ belongs includes the function $w_2(r) = r$, for which the integral $\int w_2 \mathcal{L} w_2 \, dr$ is equal to $\int r^2 W(r) dr$, which may be positive even though no

bound state exists.[10] Of course, the variational principle is still valid. It may be written

$$A^{-1} \approx A_t^{-1} + \int u_{2t} \mathcal{L} u_{2t} \, dr \quad , \tag{2.8}$$

with

$$\begin{aligned} u_{2t}(C) &= 0 \\ u_{2t}(r) &\to 1 - r/A_t \quad , \quad \text{for } r \to \infty \quad . \end{aligned} \tag{2.9}$$

It may be mentioned that if no bound state exists and if A is positive, it is possible, on the basis of an application of the Kato method, to say more about Eq. (2.8), namely that it provides a lower bound on A^{-1}; no bound need be obtained from Eq. (2.8) if A is negative.[11] While this additional result can presumably be derived using the present method as well, it is apparently much simpler to deduce it from the Kato formalism where direct use can be made of the Levinson theorem.

Although Eq. (2.8) need not provide a bound, it is clear that the results of those calculations which have been performed with this variational principle can be converted into a form corresponding to the Kohn principle so that a bound can be obtained. Thus, if A_t^{-1} and

$$I_2 \equiv \int u_{2t} \mathcal{L} u_{2t} \, dr$$

have been evaluated, we have, if we choose $u_{1t} = A_t u_{2t}$,

$$A_t^2 I_2 = \int u_{1t} \mathcal{L} u_{1t} \, dr \quad ,$$

and we may write

$$A \leq A_t - A_t^2 I_2 . \tag{2.10}$$

If A_t is positive and if $|A_t I_2|$ is small compared to unity, this conversion, in addition to providing a bound, will also provide an <u>improved</u> approximation to the true scattering length[12]. In any case this conversion does <u>not</u> provide the best result obtainable from Eq. (2.4) for a given form of the trial function since the optimum method for determining the parameters in the trial function, which is given by Eqs. (2.6), has not been employed. We thus sacrifice some accuracy in order to be able to utilize, with a minimum of effort, calculations which have already been performed. Actually, as we shall shortly see, it will often be possible to choose the best value of one of the parameters, A_t, while readily utilizing other calculations.

Since a number of variational calculations have appeared in which an inside wave function[9,13] is employed, it is useful to reexpress the preceding results in a form which contains such a function explicitly. To do this, we write the function u_{1t} as

$$u_{1t}(r) = - A_t y(r) + A_t - r , \tag{2.11}$$

where

$$\begin{aligned} y(0) &= 1 , \\ y(r) &\to 0 , \qquad \text{for } r \to \infty , \end{aligned} \tag{2.12}$$

with $y(r)$ independent of A_t. Equation (2.4) now takes the form[14]

$$A \leq A_B - 2BA_t - CA_t^2 \quad , \tag{2.13}$$

where

$$A_B = -\int W(r)\, r^2 dr \quad ,$$

$$B = \int W(r)\, r(y-1)\, dr \quad , \tag{2.14}$$

$$C = \int \left[-\left(\frac{dy}{dr}\right)^2 + W(r)\,(y-1)^2 \right] dr \; ;$$

A_B is the Born approximation to the scattering length. If A_t is determined variationally, Eq.(2.13) becomes

$$A \leq A_B + B^2/C \tag{2.15}$$

Since C must be negative (the right hand side of Eq. (2.13) is bounded from below), the bound obtained from Eq. (2.15) is an improvement over A_B. This is an example of the special property, mentioned previously, which the Kohn principle assumes in the case of zero energy scattering with no bound state, namely that a more flexible trial function must lead to an improved result.

If Eq. (2.8) is used, the trial function may be written

$$u_{2t}(r) = -y(r) + 1 - r/A_t \quad .$$

Here y(r) need not be identical to the y(r) which appears in Eq. (2.11) but is chosen to satisfy the same boundary conditions. The analogue to Equation (2.15) is then

$$A^{-1} \approx A_B^{-1}\,(1 + B)^2 + C \quad , \tag{2.16}$$

where A_B, B, and C are given by Eqs. (2.14). This is just the zero energy form of the variational principle given by Rubinow[15]. For those calculations that have been performed using the Rubinow principle, the results may be reanalysed by rearranging the known quantities A_B, B, and C according to Eq. (2.15). A consistency check on the calculation may be obtained by comparing the two variational approximations to A; if the trial function is an accurate one, the two results should differ by only a second order quantity. Further, if no bound state exists, Eq. (2.15) will provide a bound on A while Eq. (2.16) need not do so in general. An example in which this conversion provides, in addition, an improved approximation to the true scattering length, for the case of n - D quartet scattering, is given in II.

It should be pointed out that we have presented two methods for converting the results of calculations based on Eq. (2.8) to those corresponding to the Kohn form, Eq. (2.4). If the integrals A_B, B, and C are known, the conversion should be made with the aid of Eq. (2.15) rather than with Eq. (2.10), since the former employs a variationally determined value for the parameter A_t which, as we have already seen, represents the optimum choice. Since the value of A_t used in Eq. (2.10) is determined by non-optimum considerations, the bound obtained in this case would not be as good.

The question naturally arises as to how one would know that no bound state exists. For the case of the static potential, one can attack this problem theoretically; for example, it is known[16] that no bound state of angular momentum L can exist if the condition

$$(2m/\hbar^2) \int |V(r)| \; r dr < (2L + 1)$$

is satisfied. Unfortunately, no such general condition is known for the many body problem. It is however perfectly permissible, for both the one body and the many body problem, to utilize the experimental information, where available, that no bound state exists.

III. ILLUSTRATIVE EXAMPLE

As an example we consider the problem of zero energy neutron-proton scattering in the singlet state, assuming a schematic potential of the form

$$\begin{aligned} V(r) &= +\infty \quad , & r < c \ , \\ &= -V_0 \quad , & c < r < b + c \ , \\ &= 0 \quad , & b + c < r \ , \end{aligned}$$

with $b = 1.9$ f and $c = 0.4$ f ($f = 10^{-13}$ cm) . The form of the potential and the values of $\underline{b}$ and $\underline{c}$ are those chosen by Gomes, Walecka and Weisskopf.[17] The potential strength, V_0, however, is not their value but is chosen to give the experimental singlet scattering length, $A = -23.75$ f ; we obtain $W_0 b^2 \equiv (2\mu/\hbar^2)\, V_0 b^2 = 2.319$. With this potential, which does not have a bound state, a calculation of the scattering length is performed using the Kohn variational principle, Eq. (2.4). The trial function is taken to be of the form

$$\begin{aligned} u_{1t}(r) &= 0 \quad , & r < c \ , \\ &= \sum_{n=1}^{3} a_n (r-c)^n \quad , & c \leq r \leq b + c \qquad (3.1) \\ &= A_t - r \quad , & r \geq b + c \ . \end{aligned}$$

The free variational parameters in the trial function were evaluated according to both the Kohn and Hulthén methods, Eqs. (2.6) and (2.7) respectively; the results are presented in Table I. While the superiority of the Kohn method over that of Hulthén is barely discernible in this simple one body problem, its recognition might very well provide a decided advantage in more complicated many body problems. In fact, an example in which the superiority of the Kohn form is significant is presented in II, where previous variational calculations for the n-D quartet scattering problem are considered.

If we renormalize the trial function by multiplying through by A_t^{-1} it may be used to obtain results corresponding to the variational principle given by Eq. (2.8). Results appear in Table I. We have previously observed (see Section II) that the variational principle, Eq. (2.8), need not in general provide an upper bound on the scattering length. This is illustrated in the present example where, with A_t^{-1} set equal to zero, the variational estimate lies below the true scattering length. While not a bound, it is actually better than the Kohn and Hulthén results obtained with one free variational parameter. If the scattering length is negative, it may be expected, with a sufficiently accurate trial function, that Eq. (2.8) will lead to lower estimates of A than those obtained from Eq. (2.4). Since these estimates are not bounds on A, no general statement can be made concerning the relative accuracy of the two variational principles, unlike the situation previously described for positive scattering lengths (see Section II).

IV. HIGHER ANGULAR MOMENTA.

The discussion in Sections II and III was confined to the case of zero orbital angular momentum. Similar results may be obtained for states of higher angular momenta. In particular, if no bound state exists in a state with orbital angular momentum quantum number L, then the Kohn variational principle gives a bound on the parameter which characterizes the asymptotic form of the zero energy partial wave of angular momentum L, $u_L(r)$. The proof, given below, is a direct generalization of that presented in Section II for the case L = 0.

The differential equation satisfied by $u_L(r)$ at zero energy is

$$\mathcal{L}u(r) \equiv \left[\frac{d^2}{dr^2} + W(r) - \frac{L(L+1)}{r^2} \right] u(r) = 0 \quad ;$$

the boundary conditions are taken to be

$$\begin{aligned} &u(0) = 0 \\ &u(r) \to -r^{L+1} + A_L \, r^{-L} \big/ (2L+1) \, , \quad \text{for } r \to \infty \, . \end{aligned} \tag{4.1}$$

The subscript L has been dropped, except on A_L, A_{Lt}, and the phase shift, η_L. The connection between A_L and η_L is given by

$$A_L = -\left[1 \times 3 \times \ldots \times (2L+1)\right]^2 \left(\tan \eta_L \big/ k^{2L+1}\right)_{k=0} \, .$$

Note that A_L has the dimensions of a length only for L = 0. We now introduce a trial function, $u_t(r)$, which satisfies the boundary conditions

$$u_t(0) = 0$$

$$u_t(r) \to -r^{L+1} + A_{Lt}\, r^{-L}/(2L+1) \quad , \quad \text{for } r \to \infty \, , \tag{4.2}$$

where A_{Lt} is an arbitrary parameter. The Kato identity for this system will now be derived. We define

$$K \equiv \int (u \mathcal{L} u_t - u_t \mathcal{L} u)\, dr \quad ,$$

and evaluate it in two ways. Since $\mathcal{L} u = 0$, we have immediately

$$K = \int u \mathcal{L} u_t dr \quad .$$

On the other hand, integration by parts gives

$$K = \left(u \frac{du_t}{dr} - u_t \frac{du}{dr}\right) \Big|_0^\infty = A_{Lt} - A_L \quad ,$$

where use has been made of Eqs. (4.1) and (4.2). If these two forms for K are equated, and the function $w \equiv u_t - u$ is introduced, the identity,

$$A_L = A_{Lt} - \int u_t \mathcal{L}\, u_t dr + \int w \mathcal{L}\, w\, dr \quad ,$$

is obtained. With the assumed normalization, w has the asymptotic form

$$w \to (A_{Lt} - A_L)\, r^{-L}/(2L+1) \quad ,$$

and is therefore quadratically integrable for $L > 0$. It then follows, without the necessity of performing any limiting processes for $L > 0$, that since no bound state exists, $\int w \mathcal{L}\, w\, dr$ is negative; the inequality

$$A_L \leq A_{Lt} - \int u_t \mathcal{L} u_t \, dr \tag{4.3}$$

therefore holds. Just as in the case for L = 0, the validity of this result depends on the chosen asymptotic form for the wave function. If, for example, we replace Eqs. (4.1) by

$$u(0) = 0 \quad ,$$

$$u(r) \to -(2L + 1) A_L^{-1} r^{L+1} + r^{-L} \quad , \quad \text{for } r \to \infty \quad ,$$

with similar boundary conditions on $u_t(r)$, then the difference function, w, increases as r^{L+1} for large r. It is not true that $\mathcal{L}$ is negative definite for functions of this type, as may be seen by considering the particular function $w = r^{L+1}$, for all r. The variational principle

$$A_L^{-1} \approx A_{Lt}^{-1} + \int u_t \mathcal{L} u_t \, dr \quad ,$$

with

$$u_t(0) = 0 \quad ,$$

$$u_t(r) \to -(2L + 1) A_{Lt}^{-1} r^{L+1} + r^{-L} \quad , \quad \text{for } r \to \infty \ ,$$

is valid nevertheless.

V. SUMMARY

The results obtained apply to the problem of the zero energy scattering of a particle from a center of force where no bound state exists. The following properties may then be attributed to various forms of the variational principle.

(1) Upper bounds on the scattering length are provided by the Kohn principle, the Hulthén principle, and the Born approximation.

(2) The prescription given by Kohn to evaluate the variational parameters (Eqs. (2.6)) should be used rather than that of Hulthén (Eqs. (2.7)) since in the former case the bound obtained lies closer to the true scattering length. It has the further advantage, not present in the Hulthén method, that the use of a more flexible trial function, which reduces to the original trial function for certain values of the parameters, guarantees an improved result.

(3) While the Rubinow formulation does not generally provide a bound under the circumstances considered, the various integrals which enter into the variational expression for the scattering length may be rearranged in such a way that a result corresponding to the Kohn form is obtained. Consequently, calculations based on the Rubinow form which have already been performed may be used to obtain a bound with only a trivial amount of additional labor required.

(4) In the more special case where the scattering length is positive and the trial function is sufficiently accurate, such that third order terms can be neglected, the conversion from the Rubinow to the Kohn form, in addition to providing an upper bound, may be expected to give an improved approximation to the true scattering length.

The extension of the present technique to the case of scattering by a compound system has been given and successfully applied to the problem of zero energy n - D quartet scattering. In particular, the prescription given in Section II for converting from the Rubinow to the Kohn form of variational principle has enabled us, by means of a reanalysis of the data of a previous calculation, to deduce, in addition to a bound, a significantly improved approximation to the true scattering length.

The further extension to the cases where composite bound states do exist has been performed. Applications to zero energy singlet e^-H scattering and to doublet n - D scattering have been completed and will be reported on in the very near future.

TABLE I. Variational results for the neutron-proton singlet scattering length (expressed in units of 10^{-13} cm.) calculated with the trial function given by Eq. (3.1). A square well potential with an infinitely repulsive core was assumed, for which the exact scattering length, A, is -23.75×10^{-13} cm. The results in columns I and II were obtained from the variational principle given by Eq. (2.4); those in column III were obtained, with an appropriately altered trial function, from Eq. (2.8). In agreement with the discussion in the text, these results, for each row, satisfy the relations I > II > A; III may lie above or below A.

Free Parameters	I Hulthén	II Kohn	III
one	-19.46	-19.49	-25.55
two	-23.670	-23.671	-23.67

References, Footnotes

1. L. Spruch and L. Rosenberg, submitted for publication to the Physical Review.

2. W. Kohn, Revs. Mod. Phys. 26, 292 (1954);
T. Kikuta, Progr. Theoret. Phys. 12, 225 (1954); 12, 234 (1954);
J. Keller, Nuovo Cimento 5, 1122 (1957);
I. C. Percival, Proc. Phys. Soc. 70, 494 (1957).

3. T. Kato, Progr. Theoret. Phys. 6, 295 (1950);
6, 394 (1951); Phys. Rev. 80, 475 (1950). For some extensions and refinements of the method, see L. Spruch and M. Kelly, Phys. Rev. 109, 2144 (1958), and L. Spruch, Phys. Rev. 109, 2149 (1958).

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5. W. Kohn, Phys. Rev. 74, 1763 (1948).

6. The theorem states that for the zero energy, zero orbital angular momentum scattering of a particle by a center of force, the phase shift is $n\pi$, where n is the number of bound states of zero orbital angular momentum. For the proof, see N. Levinson, Kgl. Danske Videnskab. Selskab, Mat -fys. Medd. 25, No.9 (1949).

7. P. Swan, Proc. Roy. Soc. A, 228, 10 (1955).

8. L. Hulthén, K. Fysiogr. Sällsk. Lund Föohandl. 14, No. 21 (1944).

9. S. I. Rubinow, Phys. Rev. 98, 183 (1955).

10. In general, if the asymptotic form of the true wave function is $d(A - r)$, and that of the trial function is $d_t(A_t - r)$, then the difference function has the asymptotic form $(d - d_t)r + d_tA_t - dA$; for $d = d_t$ the variational principle provides a bound on A if no bound state exists. This case is entirely equivalent to the one discussed above, with $i = 1$. The result does not hold in general for $d \neq d_t$.

11. Kato has given a one parameter family of variational principles for arbitrary scattering energy. For zero orbital angular momentum it takes the form

$$k \cot(\eta - \theta) \approx k \cot(\eta_t - \theta) - \int u_{\theta t} \, \mathcal{L} u_{\theta t} \, dr$$

with

$$u_{\theta t}(0) = 0 \quad ,$$

$$u_{\theta t}(r) \to \sin(kr + \eta_t)/\sin(\eta_t - \theta) \ , \quad \text{for } r \to \infty \ .$$

(This notation differs slightly from that used in the papers of Kato, where a bar serves to distinguish between exact and trial values). The normalization parameter, θ, satisfies the relation $0 \leq \theta < \pi$. For non-zero energies the Kohn form follows from the choice $\theta = \pi/2$. At zero energy, it is obtained for <u>any</u> non-vanishing value of θ; Eq. (2.8) corresponds to the choice $\theta = 0$. According to the Kato formalism, in order that the variational principle provide a bound (i.e., in order that the Kato eigenvalue, β_θ, be infinite) it is necessary that η be less than θ. From Levinson's theorem, $\eta \to 0$ as $k \to 0$ if no bound state exists. If $\eta \to 0$ from above (i.e., if $A < 0$), then normalization with $\theta = 0$ must be excluded if a bound is to be obtained.

12. See Section 3 of reference 4.

13. H. Feshbach and S. I. Rubinow, Phys. Rev. <u>88</u>, 484 (1952).

14. Note that if $y(r)$ contains linear variational parameters, then by virtue of the appearance of A_t as a factor in Eq. (2.11), Eq. (2.13) is not a quadratic form in the linear parameters. In this case the parameters cannot be determined by solving

a set of linear equations. One could remedy this of course by redefining the linear parameters in Eq. (2.11) but one would not then obtain the form, Eq. (2.15), which we find useful to consider.

15. In a similar way, the general form of the Rubinow principle, for $k \neq 0$, may be derived from the Kato variational principle with $\theta = 0$ (see footnote 11). In fact, as Kato has already pointed out (see the third paper mentioned in reference 3), many of the variational principles which have appeared in recent years, e.g., those of Hulthén, Kohn and Schwinger, may be derived from the Kato variational principle with particular choices of the parameter θ and of the form of the trial function. Of course, each of these principles has its own particular properties which should be separately investigated. But the ability to display one variational principle containing other principles as special cases makes it easier to compare their relative merits. Further, it appears that if one wishes to generate new forms of the variational principle, the Kato form presents an ideal starting point.

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Research Reports and Publications

The following is a list of all research reports in the CX series.

CX-1	S. Borowitz	The Schwinger Variational Method for Three-Body Collisions Published - Borowitz and Friedman Phys. Rev., 89, 441 (1953). Math. Rev., 14, 756 (1953).	Apr., '52
CX-2	H. Moses	A Self-Consistent Calculation of the Dissociation of Oxygen in the Upper Atmosphere Published - Phys. Rev., 87, 628 (1952).	Apr., '52
CX-3	K. Wildermuth	A Rigorous Solution of a Many-Body Problem Published - Acta Physica Austriaca, 7, 299 (1953).	Aug. '52
CX-4	B. Friedman and E. Ger	Scattering Problems in Nonrelativistic Quantum Mechanics. Part I- One Particle in One Dimension	Dec. '52
CX-5	H. Moses	Exchange Scattering in a Three-Body Problem Published - Phys. Rev., 91, 185 (1953). Math. Rev., 16, 1186 (1955).	Jan.,'53
CX-6	H. Moses	Formulation of the Kohn-Hulthén Variational Principle in Terms of the Scattering Operator Formalism Published - Phys. Rev., 92, 817 (1953). Math. Rev., 15, 587 (1954).	Apr., '53
CX-7	H. Boyet and S. Borowitz	A Variational Calculation of the Elastic Scattering of Electrons by Hydrogen Atoms Published - Phys. Rev., 93, 1225 (1954).	Apr.,'53
CX-8	H. Moses	A Self-Consistent Calculation of the Dissociation of Oxygen in the Upper Atmosphere. Part II-Three Body Recombinations Published - Phys. Rev., 91, 1408 (1953).	Apr.,'53

CX-9	E. Bauer and Ta-You Wu	The Origin of the E-Layer of the Ionosphere Published - Phys. Rev., 92, 1101 (1953).	July,'53
CX-10	J.B. Keller	Derivation of the Bohr-Sommerfeld Quantum Conditions from an Asymptotic Solution of the Schrödinger Equation Published - Annals of Physics, 4, 180 (1958).	July,'53
CX-11	E. Bauer	Self-Consistent Field Equations for H_2 and H_3	Aug.,'53
CX-12	H. Moses	The Scattering Operator in Quantum Mechanics. Part I - The Properties of the Scattering Operator from the Time-Dependent Schrödinger Equation (see CX-13) Math. Rev., 16, 1186 (1955).	Oct.,'53
CX-13	H. Moses	The Scattering Operator in Quantum Mechanics. Part II - The Scattering Operator Formalism and Other Formalisms Published - (CX-12 and CX-13, portion of the material) Phys. Rev., 96, 519 (1954). Published - (CX-12 and CX-13, summary) Il Nuovo Cimento, 1, 103 (1955). Math. Rev., 16, 1187 (1955).	Dec.,'53
CX-14	E. Bauer and Ta-You-Wu	The Cooling of a Gas by Radiation Published - Proc. Phys. Soc. of London, A 67, 741 (1954).	Apr.,'54
CX-15	S. Schwebel	An Evaluation of Approximation Methods for Three-Body Scattering Problems Published - Phys. Rev., 103, 814 (1955). Math. Rev., 16, 1187 (1955). Math. Rev., 18, 701 (1957).	May,'54
CX-16	S. Borowitz	A Perturbation Calculation of the Elastic Scattering of Electrons by Hydrogen Atoms Published - Phys. Rev., 96, 1523 (1954).	June,'54

CX-17	E. Bauer	A Method of Calculating Cross Sections for Molecular Collisions Published - J. Chem. Phys., 23, 1087 (1955).	Oct.,'54
CX-18	H. Moses and I. Kay	The Determination of the Scattering Potential from the Spectral Measure Function Published - Il Nuovo Cimento, 2, 917 (1955). Math. Rev., 16, 929 (1955). Math. Rev., 17, 372 (1956).	Jan.,'55
CX-19	H. Moses and I. Kay	The Determination of the Scattering Potential from the Spectral Measure Function. Part II - Point Eigenvalues and Proper Eigenfunctions Published - Il Nuovo Cimento, 3, 66 (1956). Math. Rev., 17, 155 (1956). Math. Rev., 17, 740 (1956).	June,'55
CX-20	H. Moses and I. Kay	The Determination of the Scattering Potential from the Spectral Measure Function. Part III - Calculation of the Scattering Potential from the Scattering Operator for the One-Dimensional Schrödinger Equation Published - Il Nuovo Cimento, 3, 276 (1956). Math. Rev., 17, 489 (1956).	Sept.,'55
CX-21	E. Bauer and Ta-You Wu	Dissociative Recombination Published - Canadian J. of Phys., 34, 1436 (1956).	Oct.,'55
CX-22	S. Borowitz and M. Klein	A Perturbation Calculation of the Inelastic Scattering of Electrons by Hydrogen Atoms Published - Phys. Rev., 103, 612 (1956).	Nov.,'55
CX-23	B. Zumino	On the Formal Theory of Collisions and Reaction Processes Math. Rev., 19, 920 (1958).	Mar.,'56

CX-24	L. Spruch	On the Eigenvalues which Give Upper and Lower Bounds on Scattering Waves Published - Phys. Rev., 109, 2144 (1958). Math. Rev., 17, 1088 (1956).	Apr.,'56
CX-25	T. Kato	On the Eigenvalues of Many-Particle Systems in Quantum Mechanics Published - Comm. Pure and Appl. Math. 10, 151 (1957).	Apr.,'56
CX-26	H. Moses	The Kohn-Hulthén Variational Procedure for the Scattering Operator and the Reactance Operator. Part I - Elementary Form of the Variational Principle Published - Il Nuovo Cimento, 5, 120 (1957). Math. Rev., 18, 540 (1957). Math. Rev., 19, 1130 (1958).	June,'56
CX-27	H. Moses	The Kohn-Hulthén Variational Procedure for the Scattering Operator and the Reactance Operator. Part II- Procedures Independent of the Normalization of the Trial Functions Published - Il Nuovo Cimento, 5, 144 (1957). Math. Rev., 18, 540 (1957).	July, '56
CX-28	E. Bauer	Coupling of Optic and Acoustic Modes of Vibration in Crystals Published - J. Chem. Phys., 26, 1440 (1957). Math. Rev., 18, 612 (1957).	Sept.,'56
CX-29	H. Greenberg and S. Borowitz	A Variational Calculation of the Scattering Cross Section for Nearly Zero Energy Electrons by Hydrogen Atoms Published - Phys. Rev., 108, 716 (1957). Math. Rev., 19, 612 (1958).	Apr.,'57
CX-30	L. Spruch	Bounds on Scattering Phase Shifts Published - Phys. Rev., 109, 2149 (1958).	May,'57
CX-31	M. Salkoff and E. Bauer	Excitation of Molecular Vibration by Collision Published - J. Chem. Phys., 29, 26 (1958).	July,'57

CX-32	I. Kay and H. Moses	The Determination of the Scattering Potential from the Spectral Measure Function. Part IV - 'Pathological' Scattering Problems in One Dimension Il Nuovo Cimento, 5, 230 (1957).	Sept.,'57
CX-33	E. Bauer	Quantum Theory of Chemical Reaction Rates	Mar.,'58
CX-34	R. Akerib and S. Borowitz	The Application of the Impulse Approximation to the Inelastic Scattering of Electrons by Hydrogen Atoms	July,'58
CX-35	C.D. LaBudde and R. Sahni	The Evaluation of Two and Three-Center Integrals Arising in Calculations on Molecular Structure Accepted - J. Chem. Phys.	Sept.,'58
CX-36	H.E. Moses and S.F. Tuan	Potentials with Zero Scattering Phase Published - Il Nuovo Cimento, 13, 197 (1959).	Nov.,'58
CX-37	K. Omidvar	Non-Adiabatic Treatment of Elastic Scattering of Electrons by Atomic Hydrogen	Jan.'59
CX-38	S. Rubinow and J.B. Keller	Asymptotic Solution of Eigenvalue Problems Accepted - Annals of Physics	Feb.,'59
CX-39	S. Rubinow	Effective Two-Body Method for Two-Electron Atoms	Feb.,'59
CX-40	L. Spruch and S. Rubinow	Low Energy Scattering by a Compound System: Positrons on Hydrogen Submitted - Phys. Rev.	Feb.,'59
CX-41	P. Walsh and S. Borowitz	The Application of Wave Functions Containing Interelectron Coordinates. I - The Ground State Energy of Lithium	Apr.,'59
CX-42	B. Rosen	Relativistic Coulomb Scattering	Apr.,'59

List of Publications not Based on Reports

S. Borowitz and B. Friedman	Three-Body Scattering Problems Phys. Rev., 93, 251 (1954).
S. Borowitz	Electron-Ion Recombination at Low Pressures Trans. AIEE, 72, Part I, 430 (1953).
H. Moses	Calculation of the Scattering Potential from Reflection Coefficients Phys. Rev., 102, 559 (1956).
J. Keller I. Kay J. Shmoys	Determination of the Scattering Potential from Scattering Data Phys. Rev., 102, 557 (1956).
J. Keller	Bounds on Phase Shifts Il Nuovo Cimento, 5, 1122 (1957).
H. Moses	Pathological Scattering in One Dimension Il Nuovo Cimento, 5, 230 (1957).
E. Bauer and Ta-You Wu	Thermal Expansion of a Linear Chain Phys. Rev., 104, 914 (1956).
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